Molecular Biology 1996 vol.30 N3 SUPPL. 2, pages 385-389

Calculation of chemical shift dispersion for α-CH protons in binase

Kivaeva L., Ibragimova G., Kutyshenko V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Crystallographic data on binase (109 aa) were used to calculate the chemical shift dispersion (CSD) for 99 α-CH protons, taking into account the effects of internal electric and magnetic fields of C=O, C-N, O-H, and aromatic rings of Phe, Tyr, and Trp. Most of the small CSDs (up to ±0.6 ppm) could be described by close sets of fitting parameters reflecting the proton microenvironment. The larger CSDs observed for α-CH protons of residues involved in secondary structure could be explained assuming that the characteristics of peptide groups (orientation of the magnetic anisotropy tensor, dipole moments) change markedly upon hydrogen bonding, and depend on the orientation and lifespan of H-bonds.

Keywords

1H NMR spectroscopy, Binase, Protein structure, Proton chemical shift